

Aspects of Localization in Ensemble Kalman Filters

Lars Nerger

Alfred Wegener Institute for Polar and Marine Research
Bremerhaven, Germany

with

P. Kirchgessner, A. Klus, A. Bunse-Gerstner
S. Losa, W. Hiller, J. Schröter, T. Janjic



BremHLR

Kompetenzzentrum für Höchstleistungsrechnen Bremen



ALFRED-WEGENER-INSTITUT
HELMHOLTZ-ZENTRUM FÜR POLAR-
UND MEERESFORSCHUNG

University of Reading, July 3, 2014

Outline

Localization – some aspects

- Choosing an optimal localization radius
- Regularizing effect
- Impact on serial observation processing (EnSRF, EAKF)

I will necessarily miss other aspects, e.g.

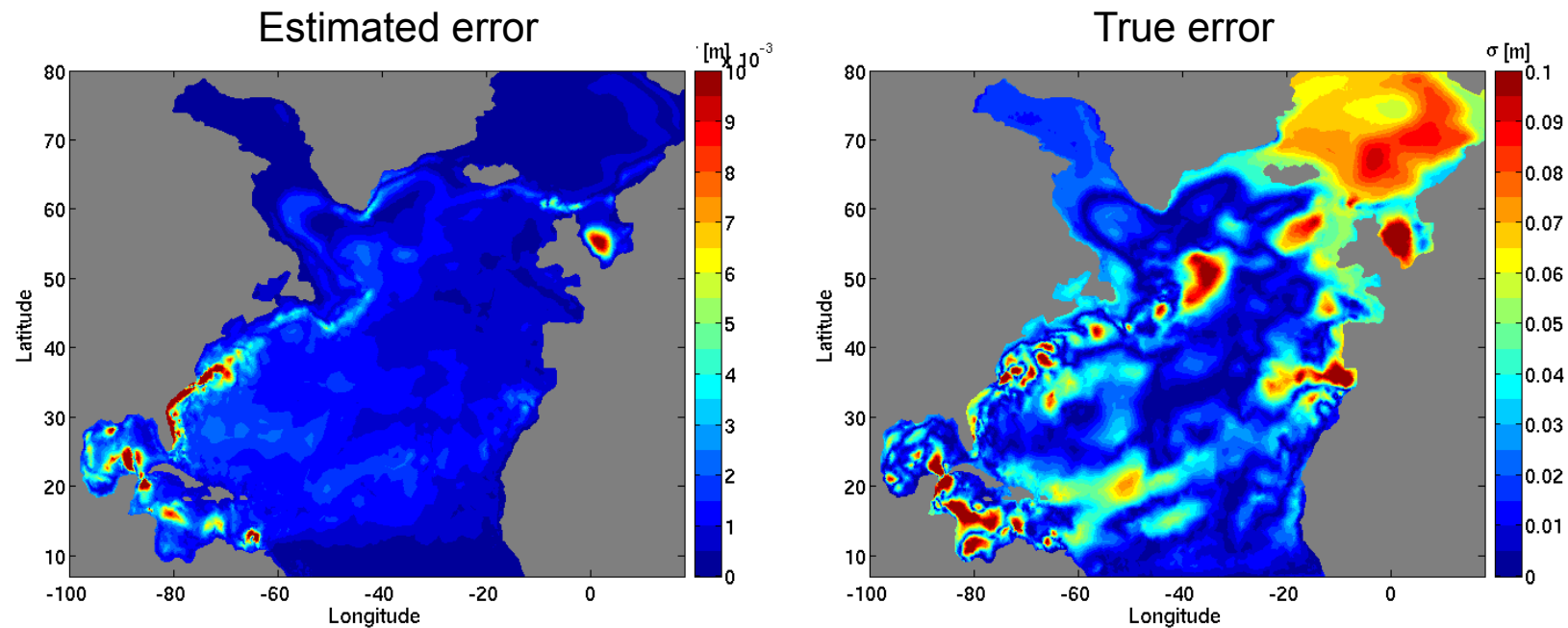
- Localization and balance
- Adaptive localization
- ...

Localization

Motivation for Localization

Ensemble Kalman filter without localization

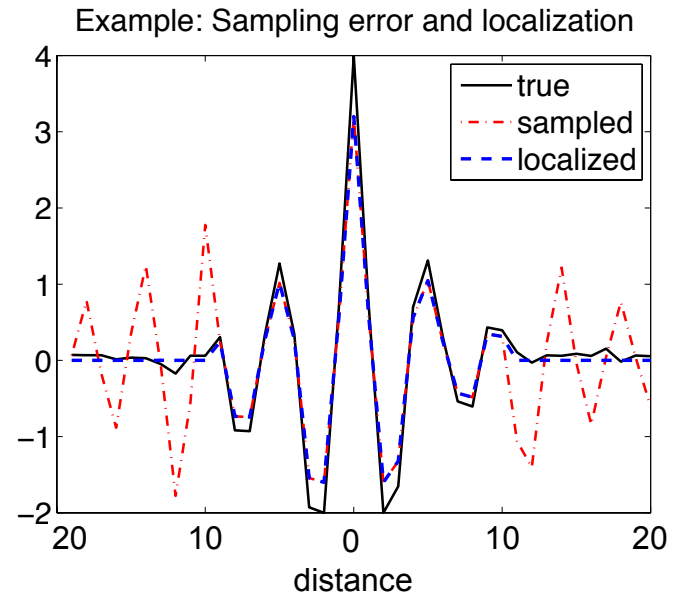
- Compute globally an optimal combination of state estimate and observations
 - small state corrections
 - strong underestimation of covariances



Example: SSH assimilation with SEIK filter and FEOM

Localization: Why and how?

- Combination of observations and model state based on ensemble estimates of error covariance matrices
- Finite ensemble size leads to significant sampling errors
 - errors in variance estimates
 - errors in correlation estimates
 - wrong size if correlation exists
 - spurious correlations when true correlation is zero
- Assume that long-distance correlations in reality are small
 - damp or remove estimated long-range correlations



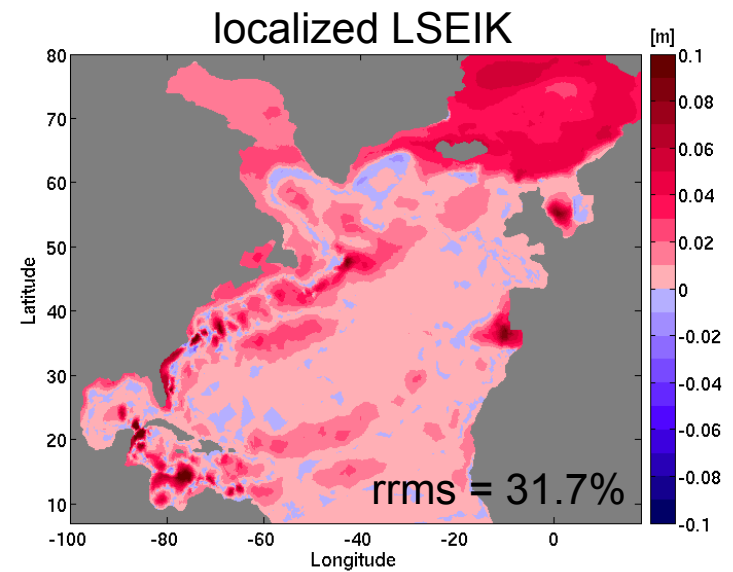
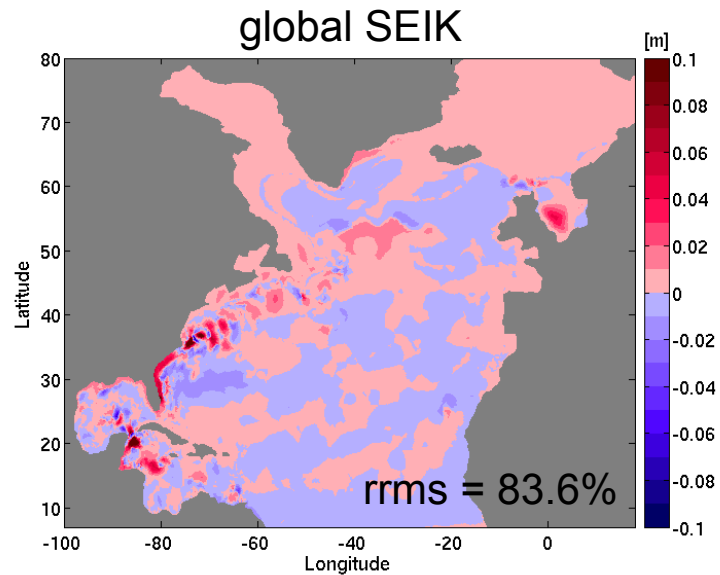
Effect of Localization

- Remove estimated long-range correlations
 - ➔ Increases degrees of freedom for analysis (globally not locally!)
 - ➔ Increases size of analysis correction
 - ➔ Reduces underestimation of analysis errors

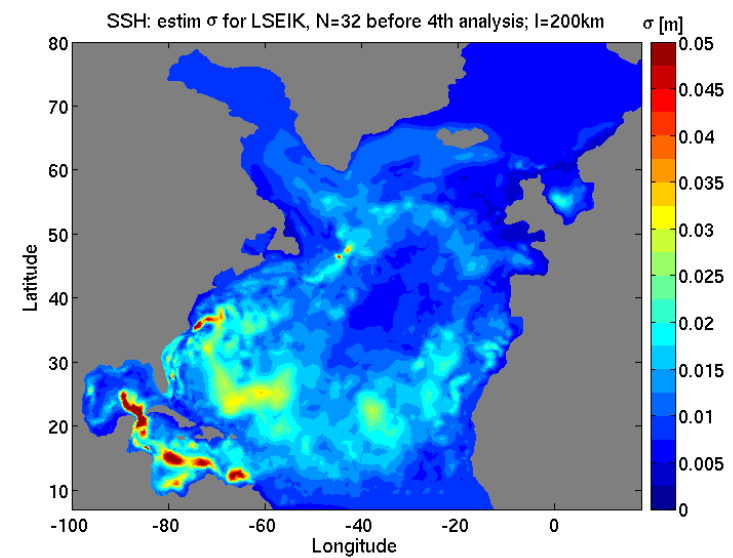
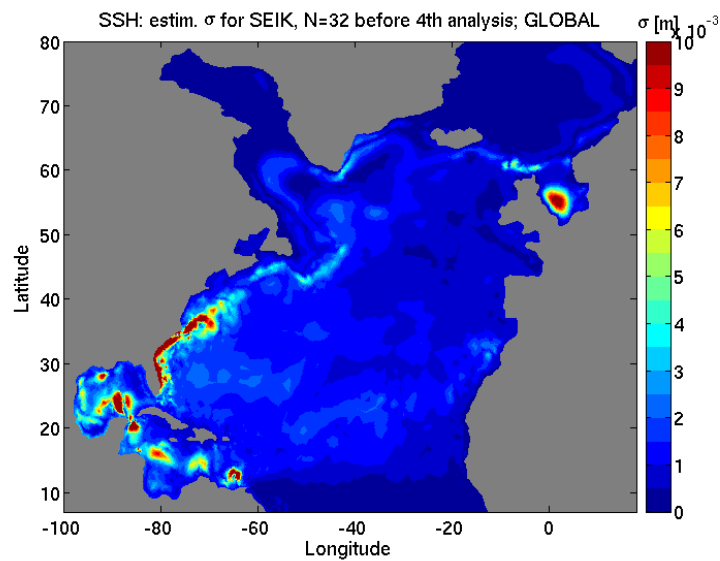
- But:
 - ➔ Also real long-range correlations are removed

Effect of Localization

Stronger
correction
of states



Large
error
estimates



Localization Types

Simplified analysis equation:

$$\mathbf{x}^a = \mathbf{x}^f + \frac{\mathbf{P}^f}{\mathbf{P}^f + \mathbf{R}} (\mathbf{y} - \mathbf{x}^f)$$

Covariance localization

- Modify covariances in forecast covariance matrix \mathbf{P}^f
- Element-wise product with correlation matrix of compact support

Requires that \mathbf{P}^f is computed
(not in ETKF, SEIK, or ESTKF)

E.g.: Houtekamer/Mitchell (1998, 2001),
Whitaker/Hamill (2002), Keppenne/
Rienecker (2002)

Observation localization

- Modify observation error covariance matrix \mathbf{R}
- Needs distance of observation (achieved by local analysis or domain localization)

Possible in all filter formulations

E.g.: Evensen (2003), Ott et al. (2004),
Hunt et al. (2007)

Domain & Observation localization

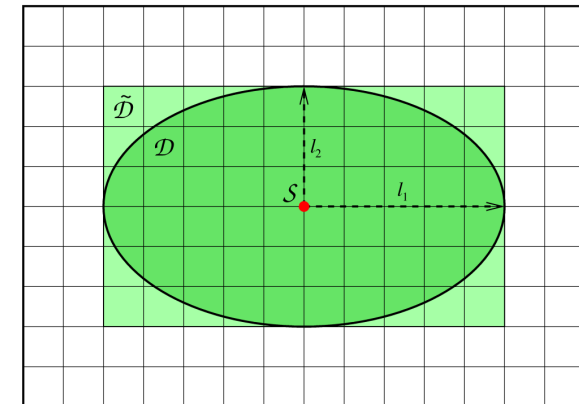
Domain localization

- Perform local filter analysis with observations from surrounding domain

Observation localization

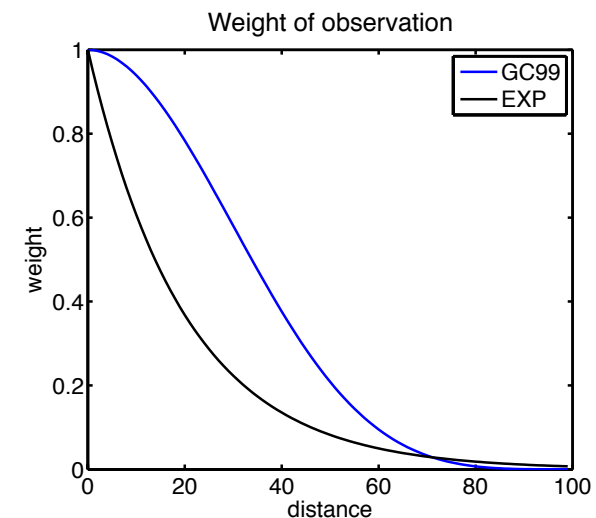
- Use non-unit weight for observations
- reduce weight for remote observations by increasing variance estimate
- use e.g. exponential decrease or polynomial representing correlation function of compact support
- similar, sometimes equivalent, to *covariance localization*

Domain Localization



S: Analysis region

D: Corresponding data region



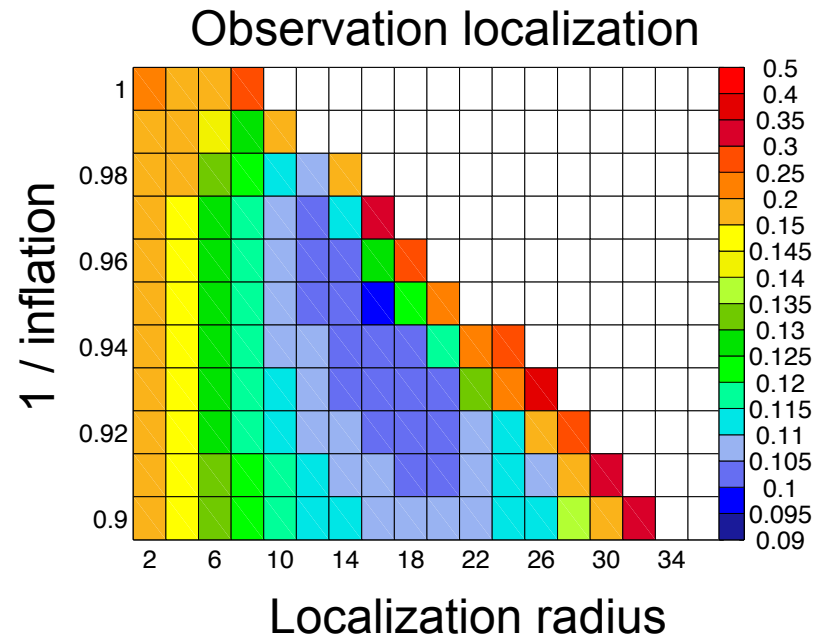
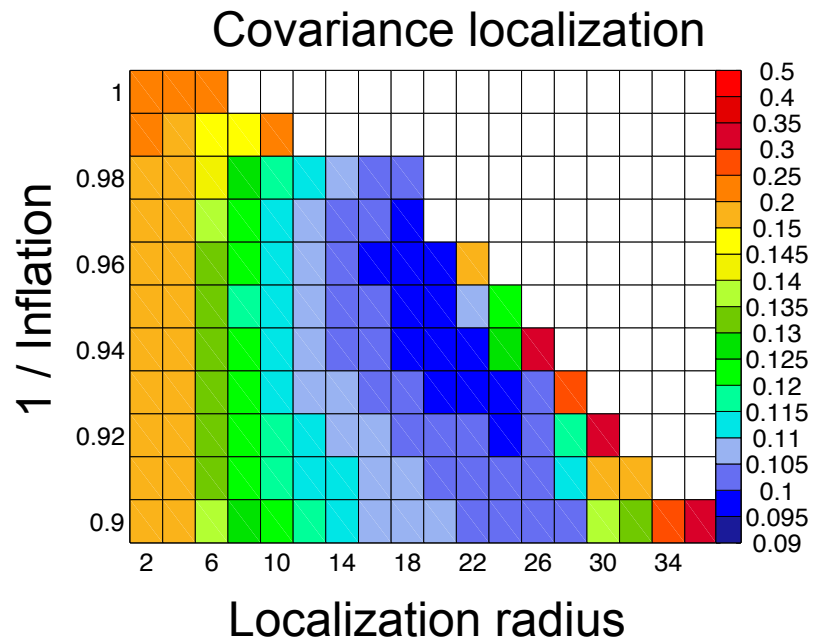
Different effect of localization methods

Experimental result:

- Twin experiment with simple Lorenz96 model
- Use a square-root EnKF and LSEIK
- Covariance localization better than observation localization
(Also reported by Greybush et al. (2011) with different model)

Time-mean RMS errors

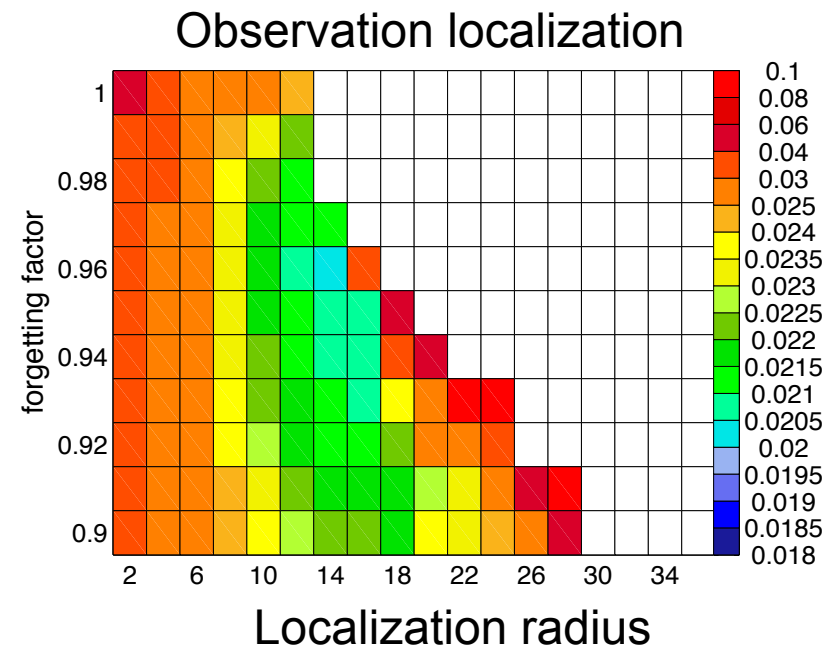
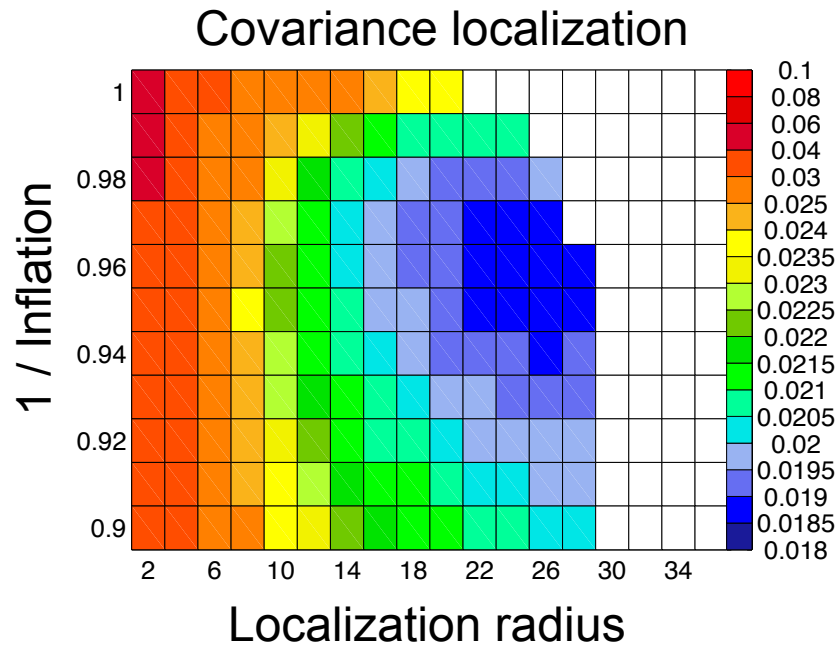
$$\sigma_R = 1.0$$



Different effect of localization methods (cont.)

Larger differences for smaller observation errors

$$\sigma_R = 0.1$$



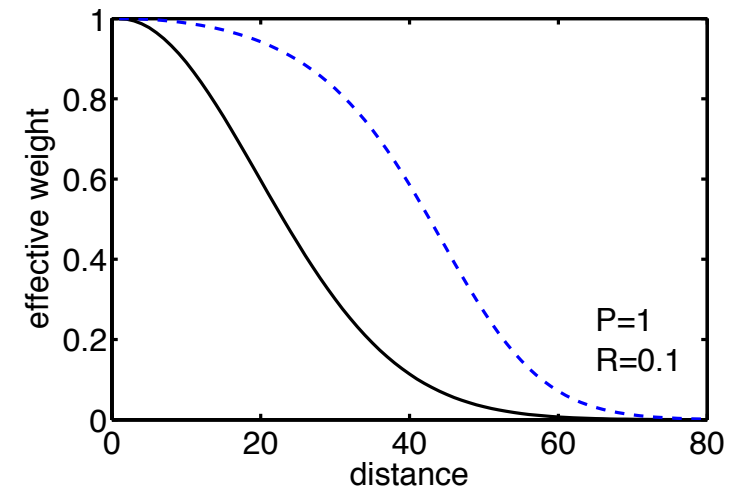
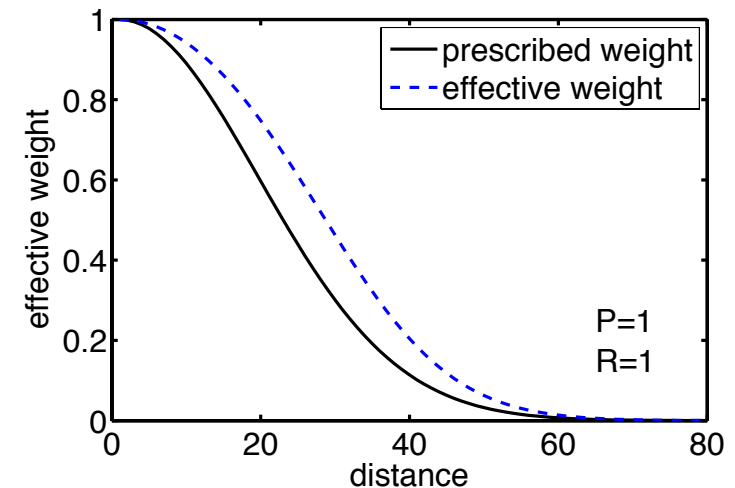
Covariance vs. Observation Localization

Some published findings:

- Both methods are “similar”
- Slightly smaller width required for observation localization

But note for observation localization:

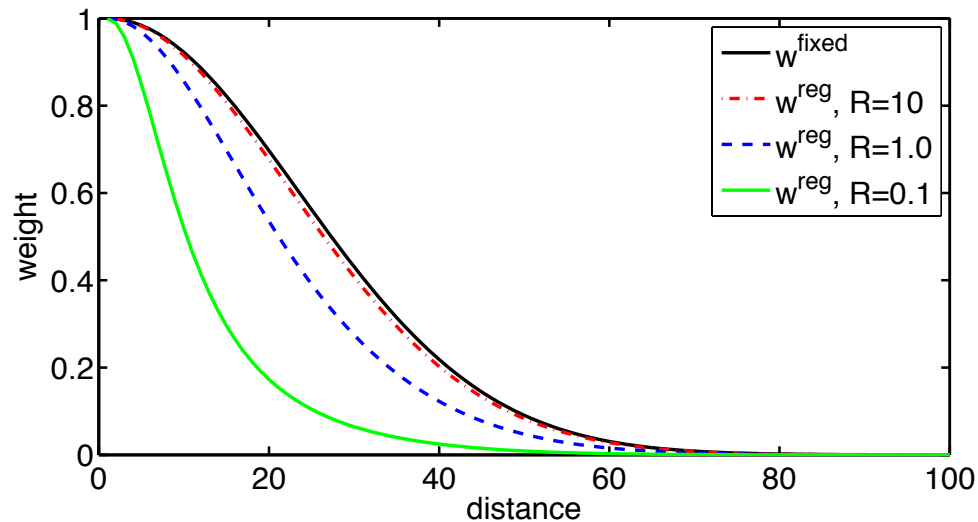
- Effective localization length depends on errors of state and observations
 - Small observation error
→ wide localization
 - Possibly problematic:
 - in initial transient phase of assimilation
 - if large state errors are estimated locally



P: state error variance
R: observation error variance

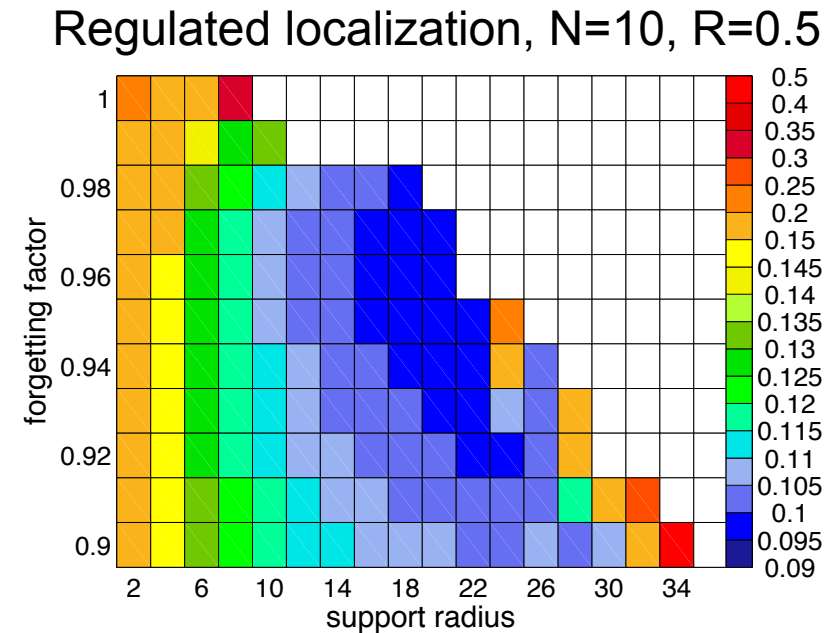
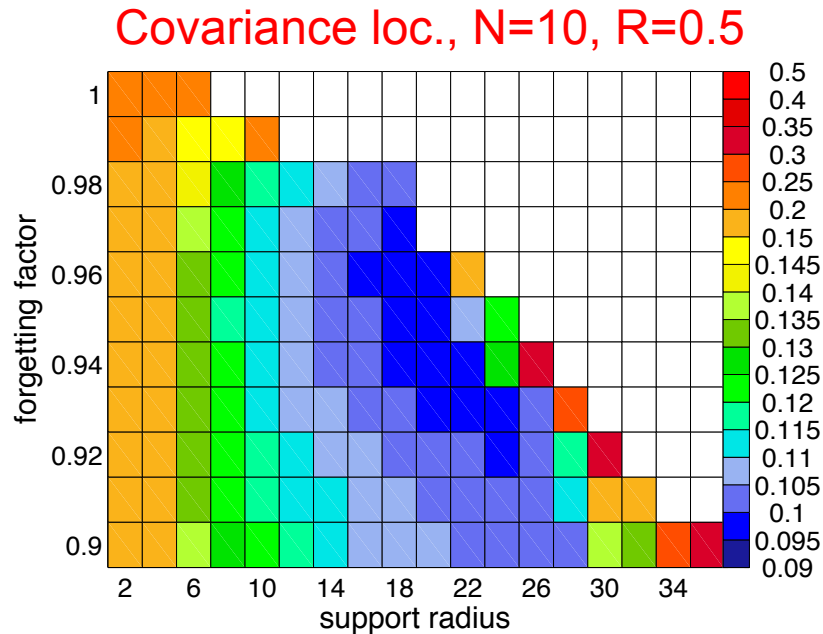
Regulated Localization

- New localization function for observation localization
 - formulated to keep effective length constant (exact for single observation)
 - depends on state and observation errors
 - depends on fixed localization function
 - cheap to compute for each observation
 - Only exact for single observation – works for multiple



P=1

Lorenz96 Experiment: Regulated Localization



- Reduced minimum rms errors
- Increased stability region
- Description of effective localization length explains the findings of other studies!
- Impact also with FESOM ocean model (but smaller)

Optimal Localization Radius

(Paul Kirchgessner et al.)

Domain & Observation localization

Localization radius can depend on

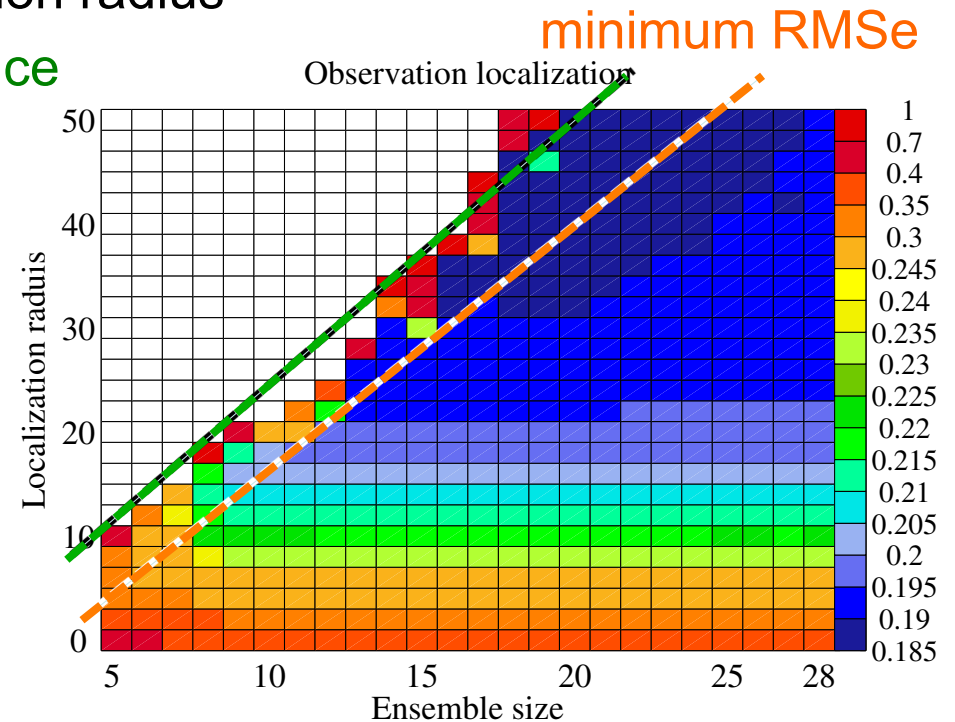
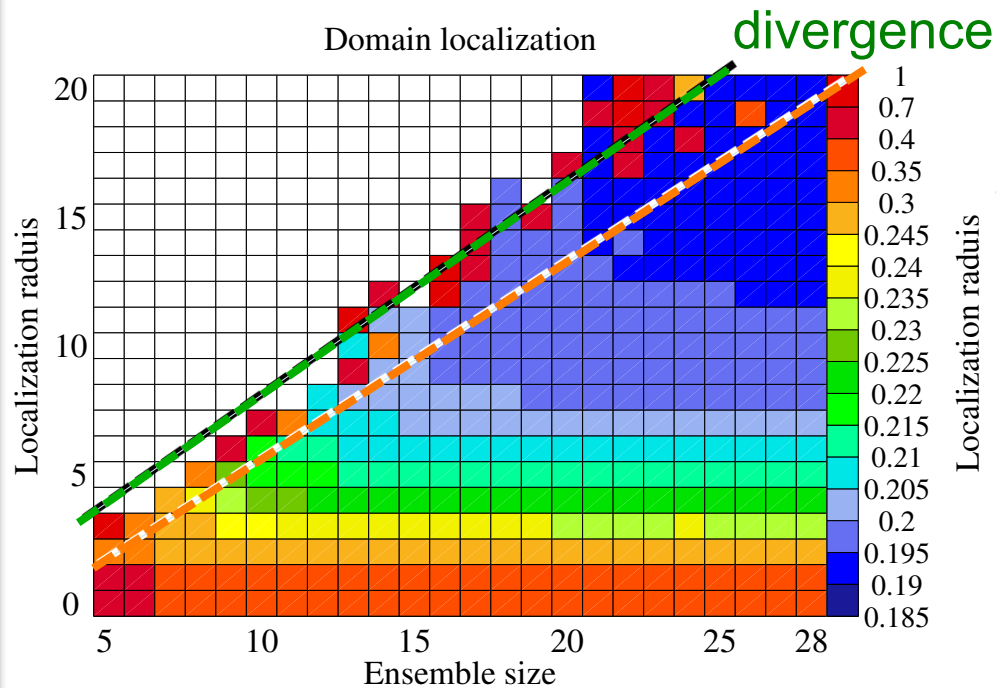
- Ensemble size
- Model dynamics & resolution
- Field

Optimal localization radius

- Typically determined experimentally (very costly)
- Some authors proposed adaptive methods (e.g. Anderson, Bishop/Hodyss)
 - still with tunable parameters

Relation between ensemble size and localization radius

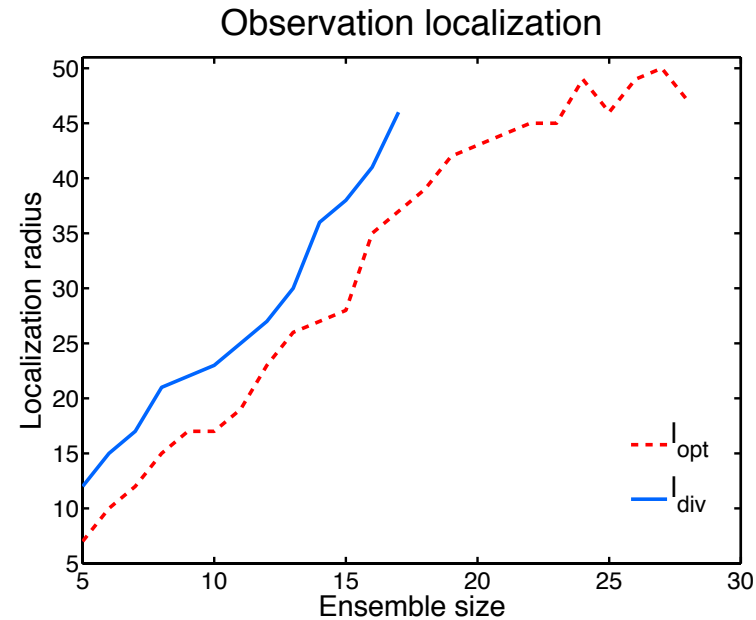
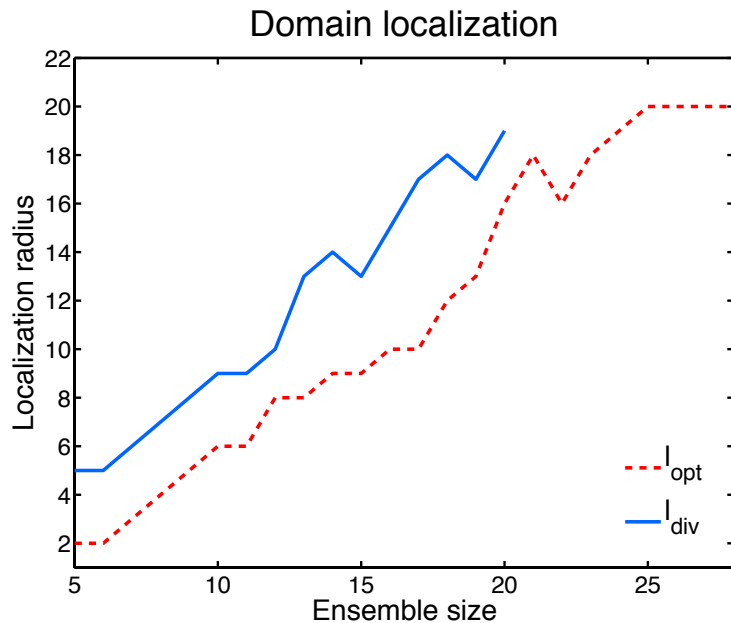
- Test runs with Lorenz-96 model
- Vary ensemble size and localization radius



- White: Filter divergence

Optimal localization radius

- Optimal localization radius as function of ensemble size

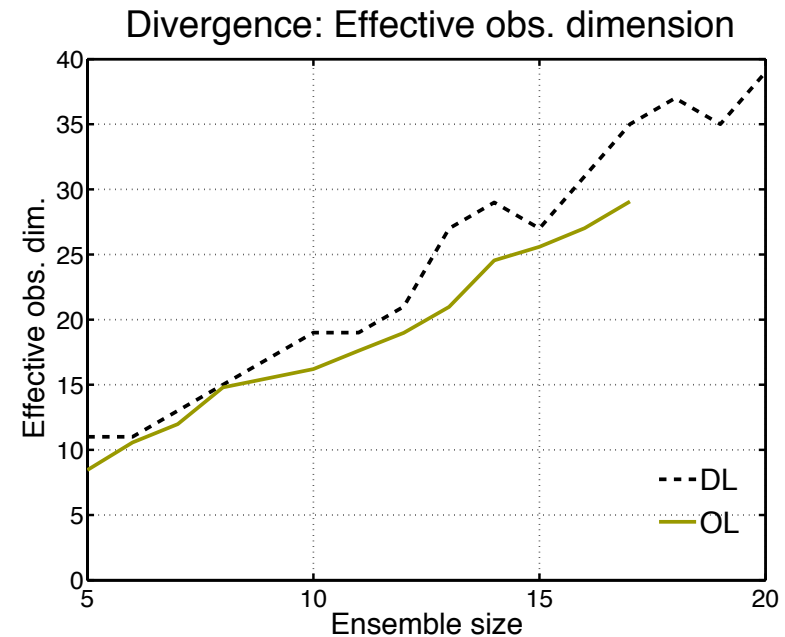
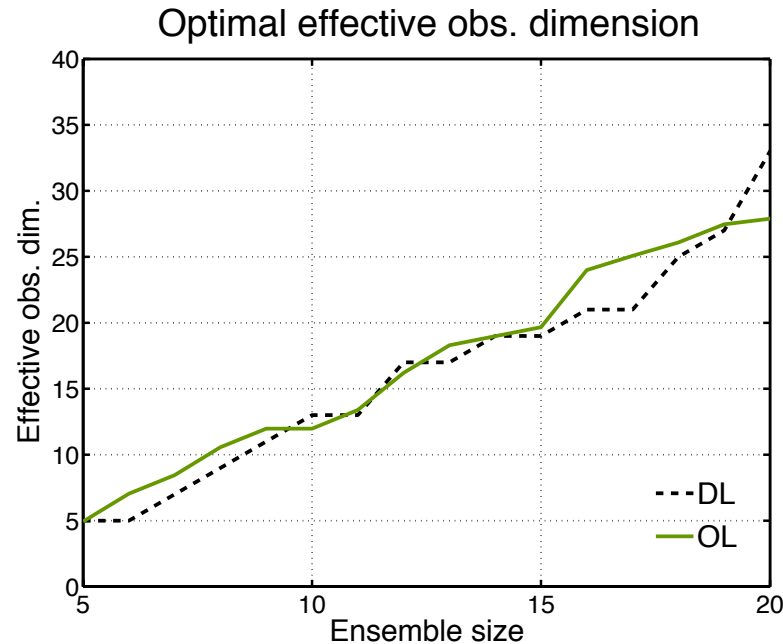


- Linear dependence for domain and observation localization
- Radius larger for OL than DL

Relate domain and observation localizations

➤ Define:

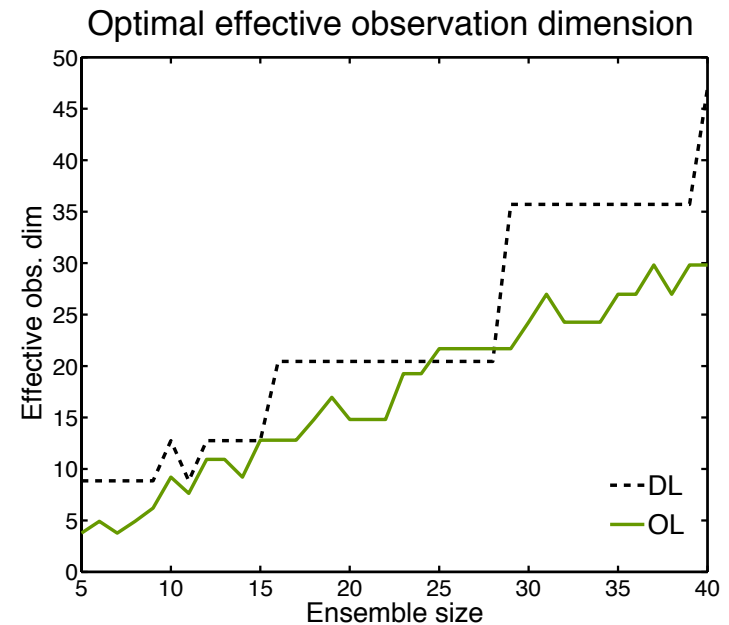
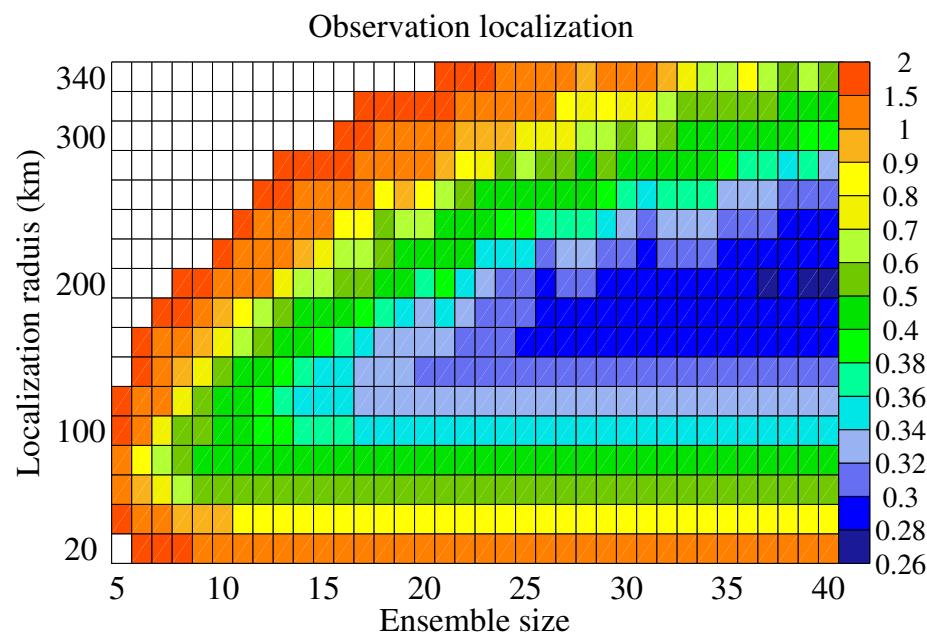
Effective observation dimension d_W = sum of observation weights



- Minimum RMS errors when effective obs. dimension slightly larger than ensemble size
- When d_W =ensemble size, errors are almost as small (optimal use of degrees of freedom from ensemble?)

2D Shallow Water Model

- Shallow water model simulating a double gyre in a box
- Assimilate sea surface height at each grid point

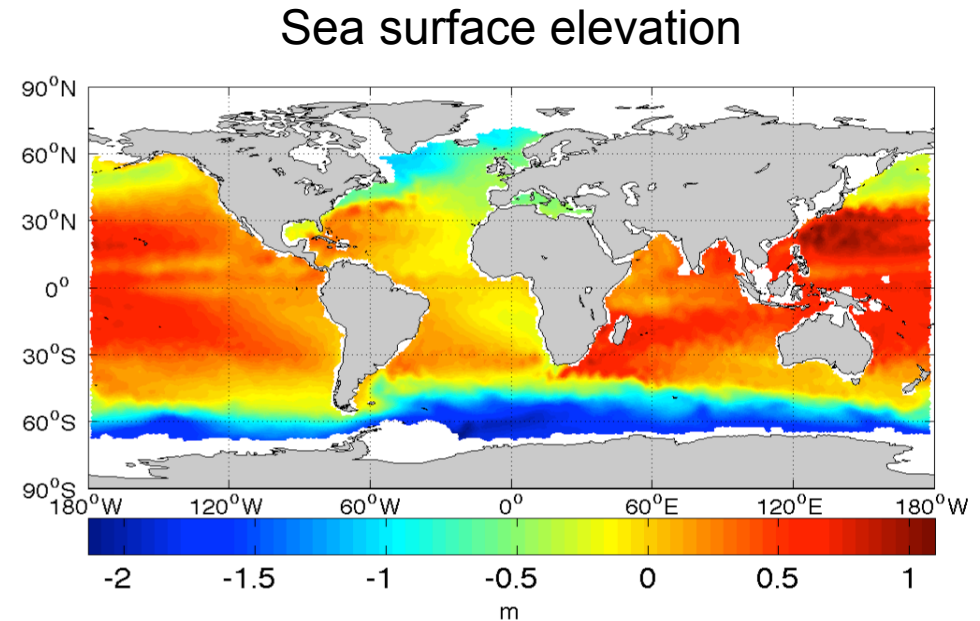


- For DL: steps due to addition of observations
- d_w optimal if about or slightly lower than ensemble size
- relation holds for different weight functions

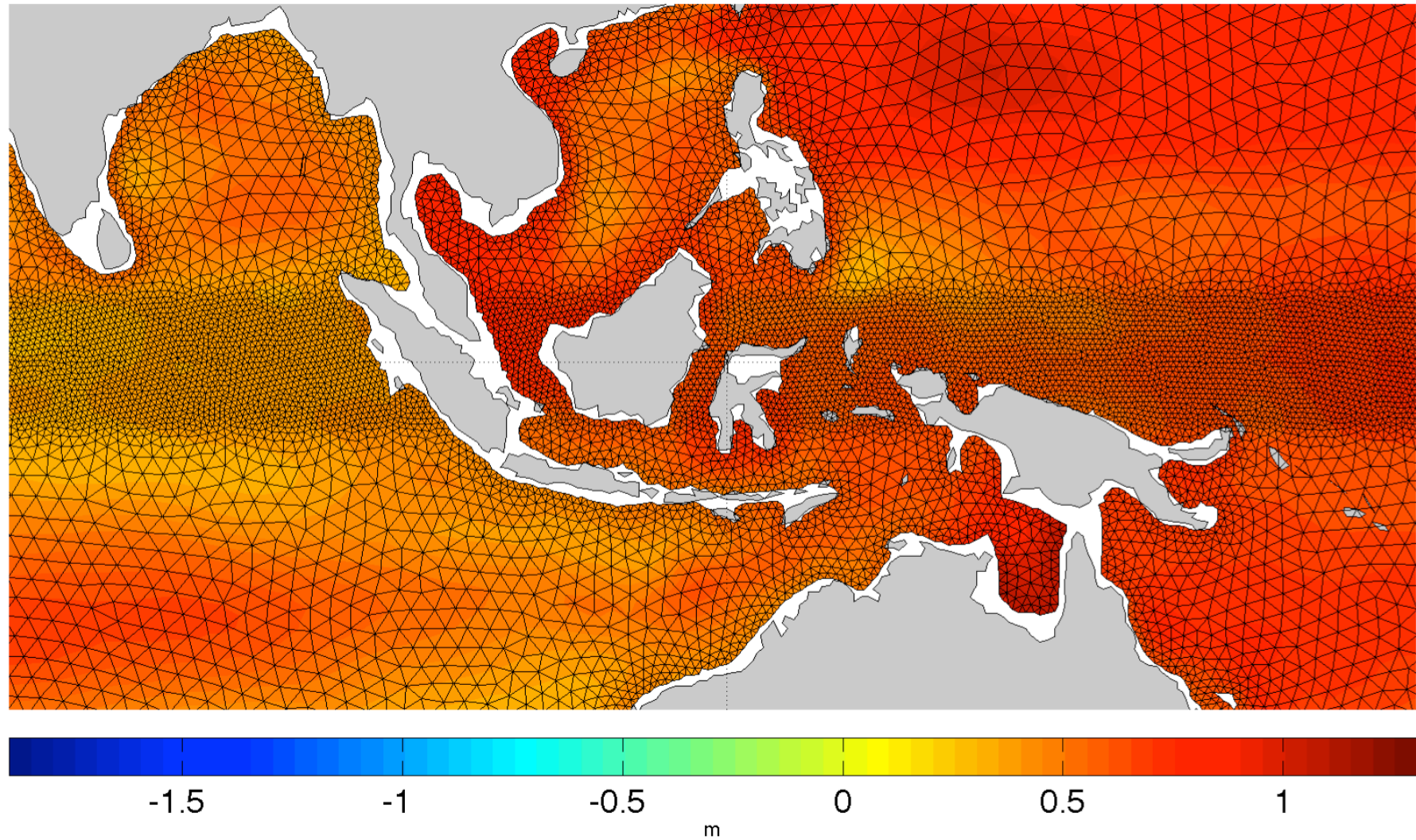
Large scale data assimilation: Global ocean model

- Finite-element sea-ice ocean model (FESOM)
- Global configuration (~1.3 degree resolution with refinement at equator)
- State vector size: 10^7
- Scales well up to 256 processor cores

- Assimilate synthetic sea surface height data for ocean state estimation
- Very costly due to large model size (using up to 2048 processor cores)



Model mesh at the equator

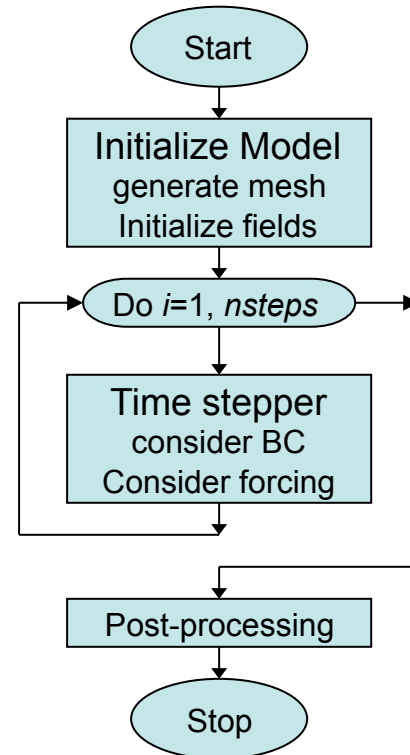


Extending a Model for Data Assimilation

PDAF

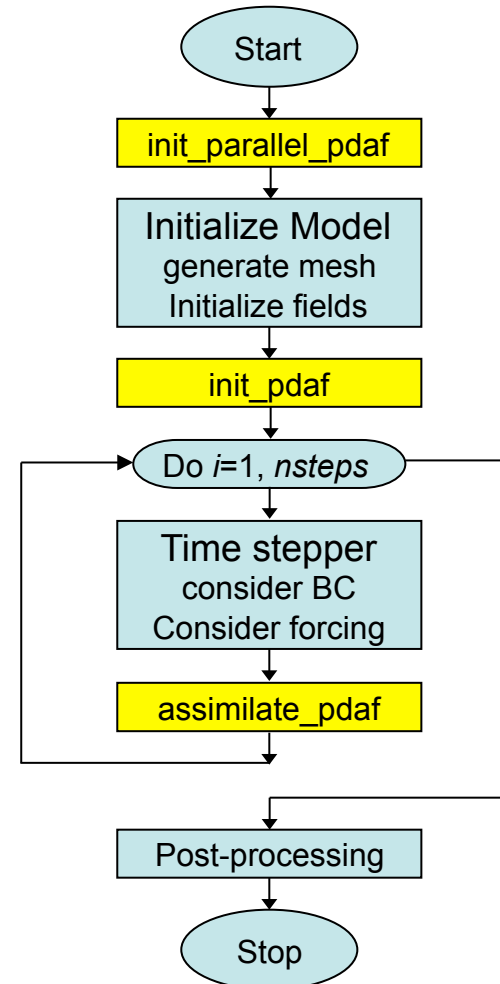
Parallel
Data
Assimilation
Framework

Model



Implementation uses parallel configuration of ensemble forecast provided by PDAF

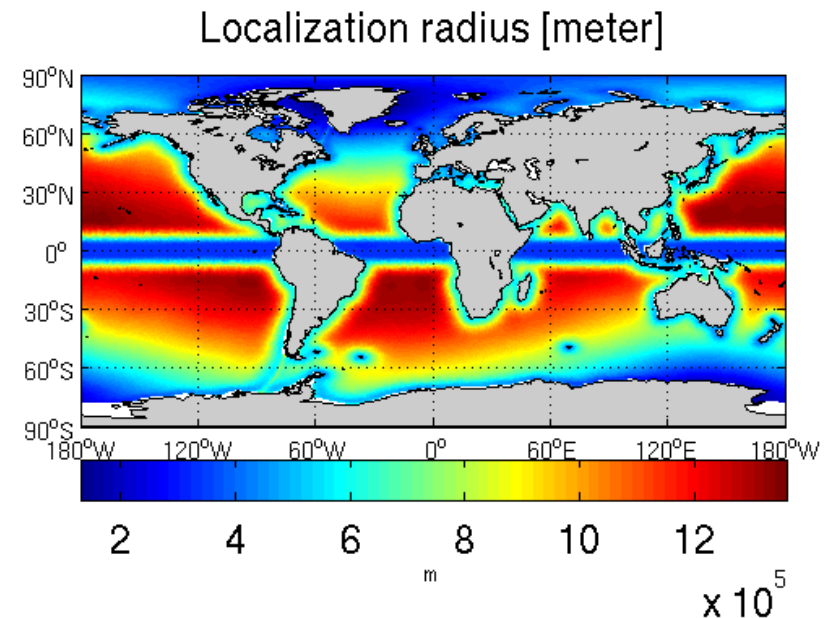
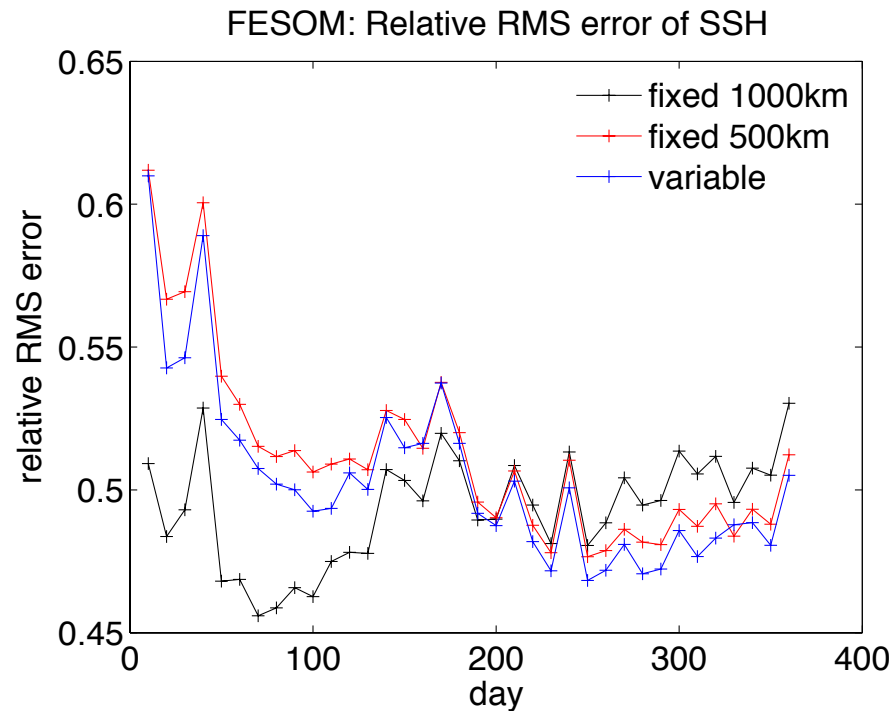
Extension for data assimilation



Open source:
Code and
documentation
available at
<http://pdaf.awi.de>

Adaptive localization radius in global ocean model

- Localization radius follows mesh resolution
- Fixed 1000km radius leads to increasing errors in 2nd half of year
- Lower RMS error in SSH than fixed 500km radius



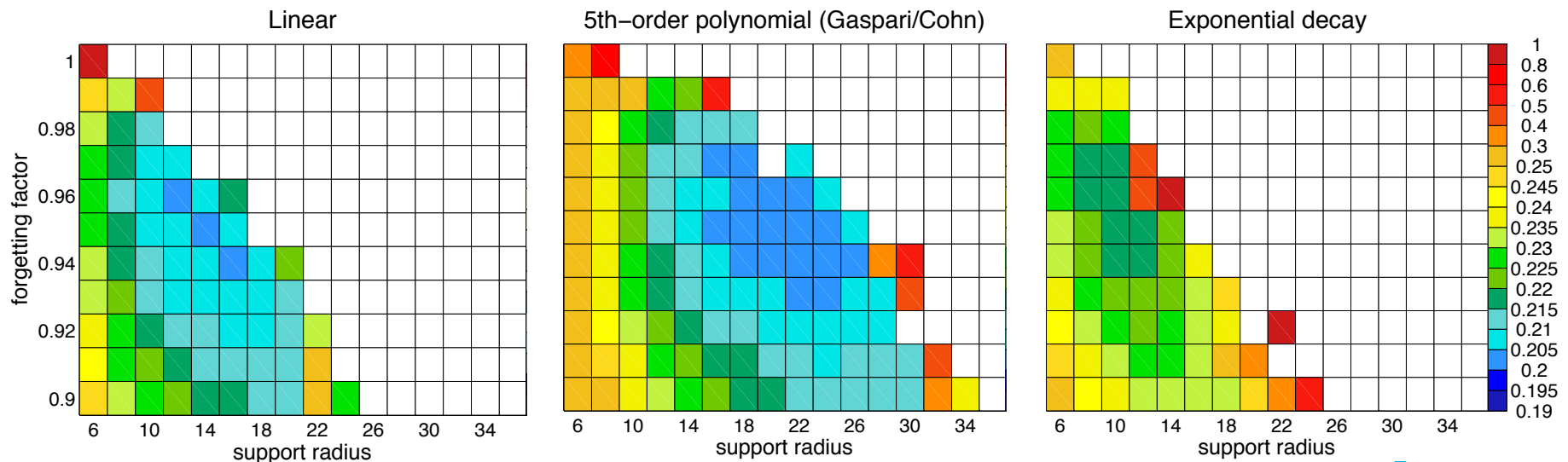
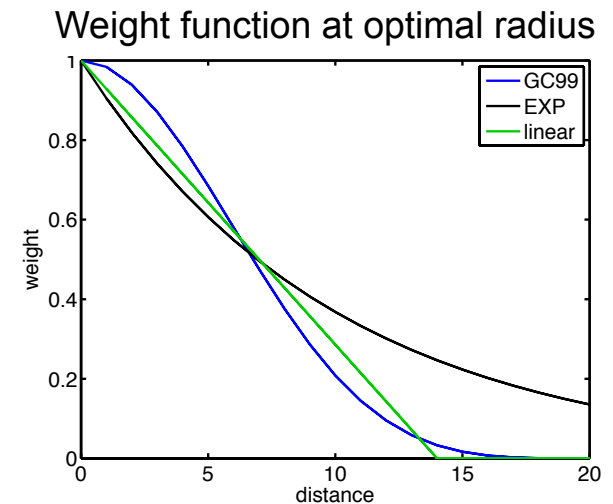
Discussion on localization radius

- Findings:
 - Effective observation dimension d_W relates to degrees of freedom
 - d_W close to ensemble size a good choice
 - No dependence on model dynamics

- Limitations
 - Observations at each grid point
(optimal d_W smaller for incomplete observations)
 - Uniform observation error
 - Ignoring information content of observations
(e.g. Migliorini, QJRMS 2013)

Weight function

- Why 5th-order Gaspari/Cohn polynomial?
- Covariance function not required for OL
- Furrer/Bengtsson (2007) indicate best sampling error reduction in \mathbf{P}^f for exponential covariances
- For Lorenz96, some other functions give similar errors – but not significantly lower ones



Localization

as Regularization

(Master thesis Andrea Klus @U Bremen)

Regularization in Ensemble Kalman Filters

- Write Kalman filter analysis as minimization

$$\|(\mathbf{P}^f)^{-1/2}\boldsymbol{\delta}\|_2^2 + \|\mathbf{R}^{-1/2}\mathbf{H}\boldsymbol{\delta} - \mathbf{R}^{-1/2}(\mathbf{y} - \mathbf{H}\mathbf{x}^f)\|_2^2 = \min!$$

with $\boldsymbol{\delta} = \mathbf{x} - \mathbf{x}^f$

- General form (not the same \mathbf{x} , \mathbf{y})

$$\|\mathbf{A}\mathbf{x} - \mathbf{y}\|_2 + \lambda\|\mathbf{L}\mathbf{x}\|_2 = \min!$$

(standard Tikhonov regularization for $\mathbf{L}=\mathbf{I}$)

- For **ETKF**

Use $\boldsymbol{\delta} = \mathbf{V}\boldsymbol{\omega}$ with $\mathbf{V}\mathbf{V}^T = \mathbf{P}^f$

then

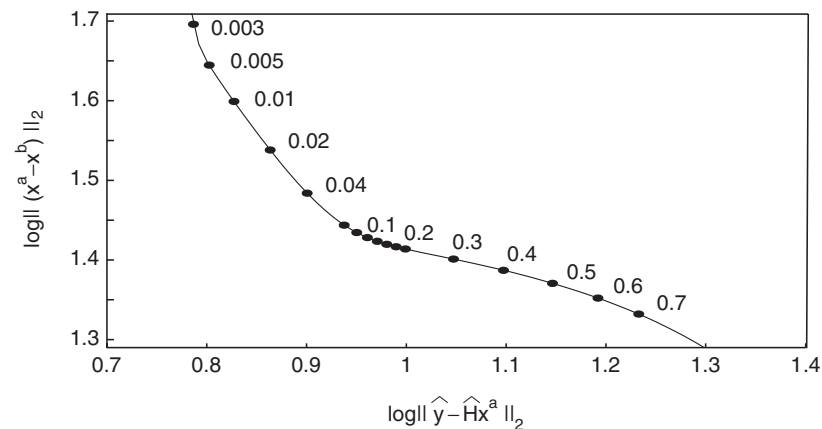
$$\|\boldsymbol{\omega}\|_2^2 + \|\mathbf{R}^{-1/2}\mathbf{H}\mathbf{V}\boldsymbol{\omega} - \mathbf{R}^{-1/2}(\mathbf{y} - \mathbf{H}\mathbf{x}^f)\|_2^2 = \min!$$

L-curves

- Examine norm of both terms on minimization problem varying λ

$$\|\mathbf{Ax} - \mathbf{y}\|_2 + \lambda \|\mathbf{Lx}\|_2 = \min!$$

- Plot residual term vs. penalty term
- Example for 4D-Var case (Johnson, Nichols, Hoskins, IJNMF, 2005)



with

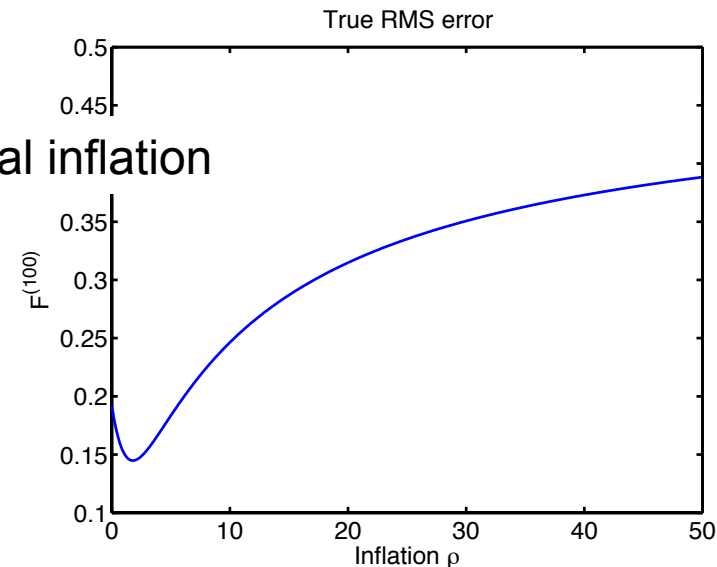
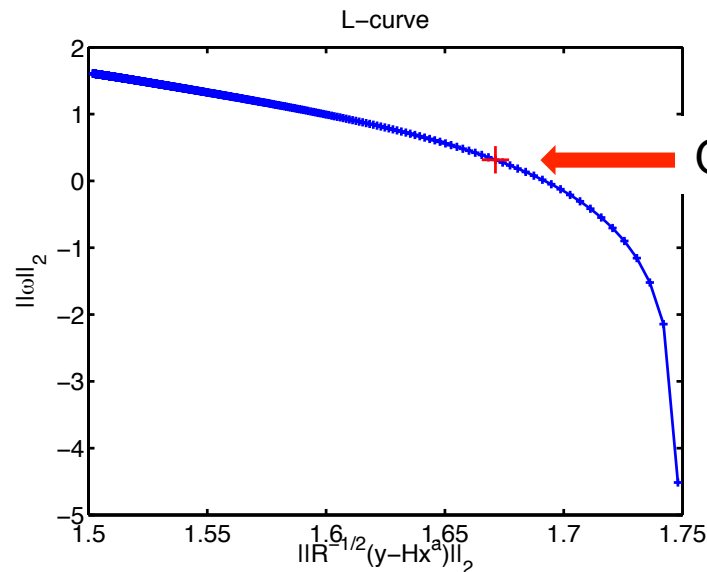
$$\tilde{\mathcal{J}}(\boldsymbol{\chi}) = \mu^2 \|\boldsymbol{\chi}\|_2^2 + \|\mathbf{C}_R^{-1/2} \hat{\mathbf{d}} - \mathbf{C}_R^{-1/2} \hat{\mathbf{H}} \mathbf{C}_B^{1/2} \boldsymbol{\chi}\|_2^2$$

ETKF with Inflation

- Inflation is a standard method to stabilize ensemble filters
- Modify minimization problem to

$$|\rho^{-1}| \cdot \|\omega\|_2^2 + \|\mathbf{R}^{-1/2} \mathbf{H} \mathbf{V} \omega - \mathbf{R}^{-1/2} (\mathbf{y} - \mathbf{H} \mathbf{x}^f)\|_2^2 = \min!$$

- L-curve (for Lorenz-96 at time step 100 and spin up with $\rho=1.05$)



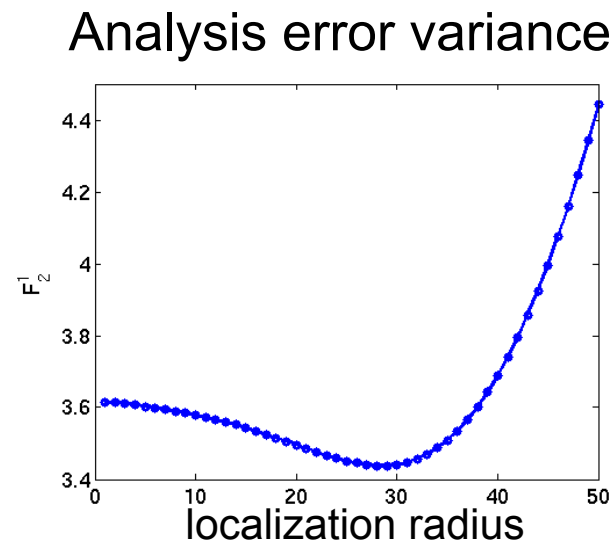
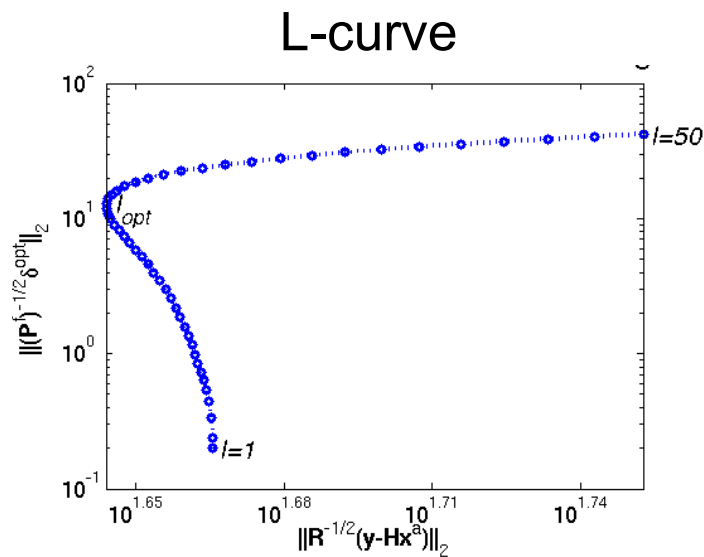
(not an 'L')

EnKF with covariance localization

- Minimize

$$\|(\mathbf{C} \circ \mathbf{P}^f)^{-1/2} \boldsymbol{\delta}\|_2^2 + \|\mathbf{R}^{-1/2} \mathbf{H} \boldsymbol{\delta} - \mathbf{R}^{-1/2} (\mathbf{y} - \mathbf{H} \mathbf{x}^f)\|_2^2 = \min!$$

- Vary localization radius l defining \mathbf{C}
- Use 5th order polynomial for \mathbf{C} (Gaspari/Cohn, 1999)

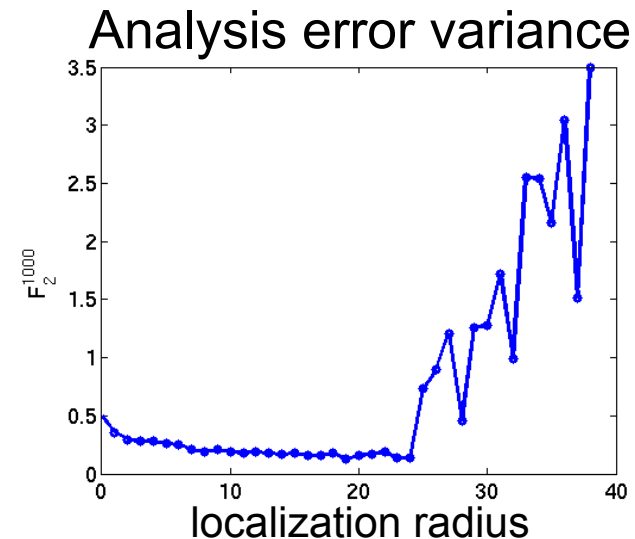
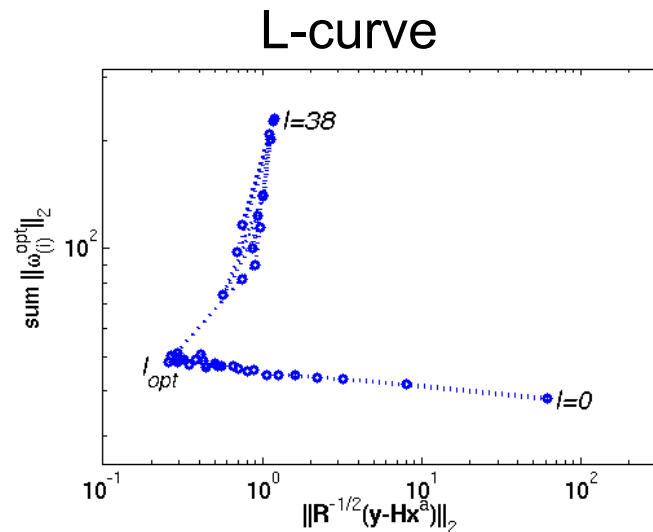


ETKF with observation localization

- Minimize the local problem

$$\begin{aligned} & \|(\tilde{\mathbf{C}}_{loc(i)} \circ (\mathbf{TR}^{-1}\mathbf{T}_i^T))^{1/2}(\mathbf{T}_i\mathbf{HV})\boldsymbol{\omega}_{loc(i)} - (\tilde{\mathbf{C}}_{loc(i)} \circ (\mathbf{TR}^{-1}\mathbf{T}_i^T))^{1/2}\mathbf{T}_i(\mathbf{y} - \mathbf{H}\mathbf{x}^f)\|_2^2 \\ & + \|\boldsymbol{\omega}_{loc(i)}\|_2^2 = \min! \end{aligned}$$

- Vary localization radius l defining \mathbf{C} and \mathbf{T}
- Consider minimization at a single grid point, sum over all points



(similar behavior at all grid points)

Discussion on regularization

- Localization regularizes the filter analysis
- Analysis for optimal radius is a posteriori
- Can we utilize it in practice?

Impact of localization

on serial observation processing

(EnSRF, EAKF)

Serial observation processing

Synchronous assimilation

ETKF, SEIK, ESTKF, (EnKF)

- Assimilation all observation at a given time at once
- Usually using ensemble-space transformations
- Possible for arbitrary observation error covar. matrices

Use

observation localization

Serial observation processing

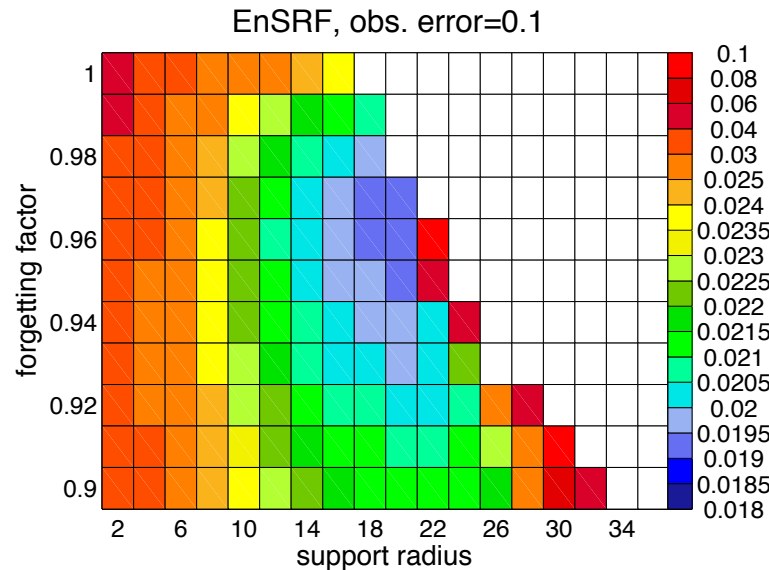
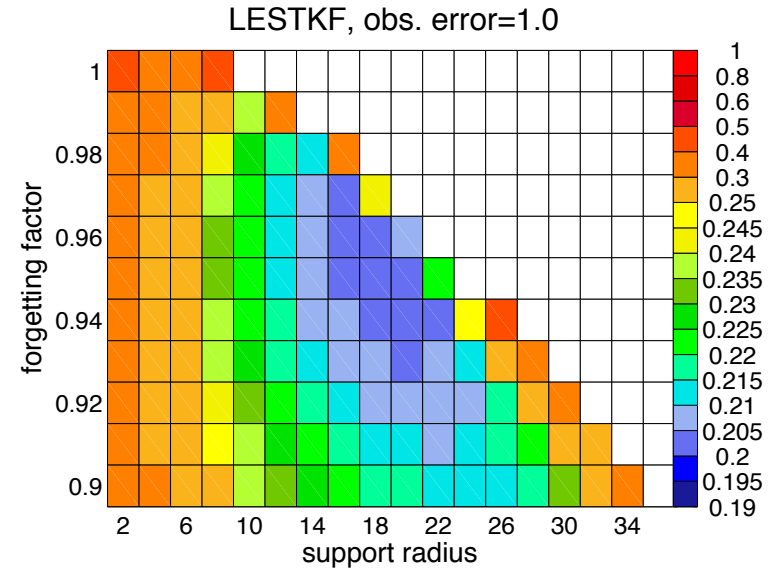
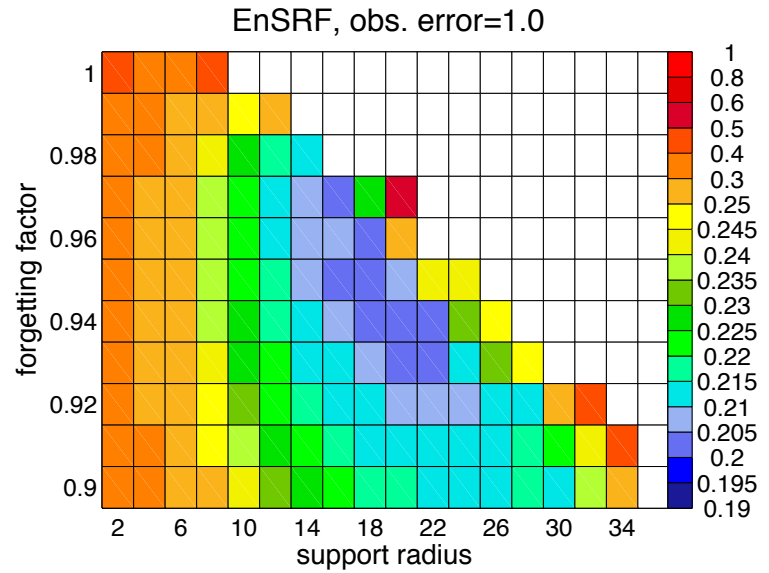
EnSRF, EAKF

- Perform a loop assimilating each single observation
- Efficient: Avoids matrix-matrix operations
- Requires diagonal observation error covar. matrix

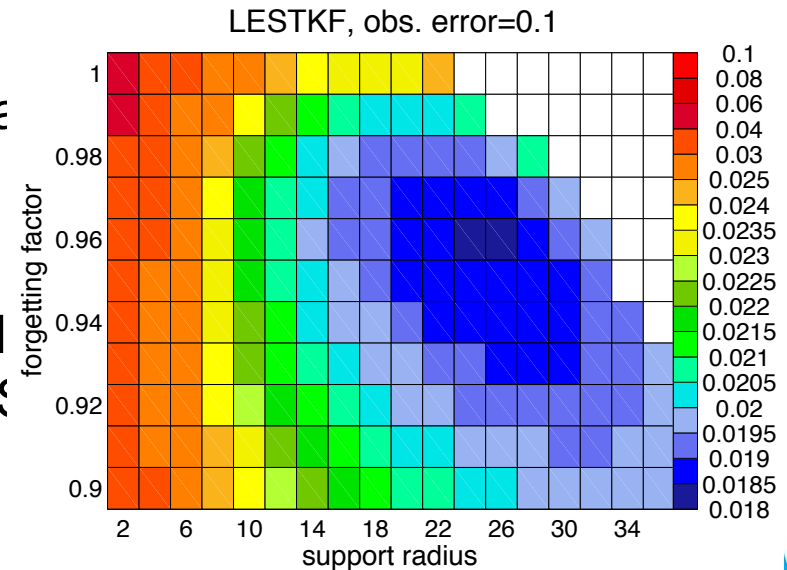
Use

covariance localization

Test with Lorenz96



Trace Tra
?)
most id
r and L

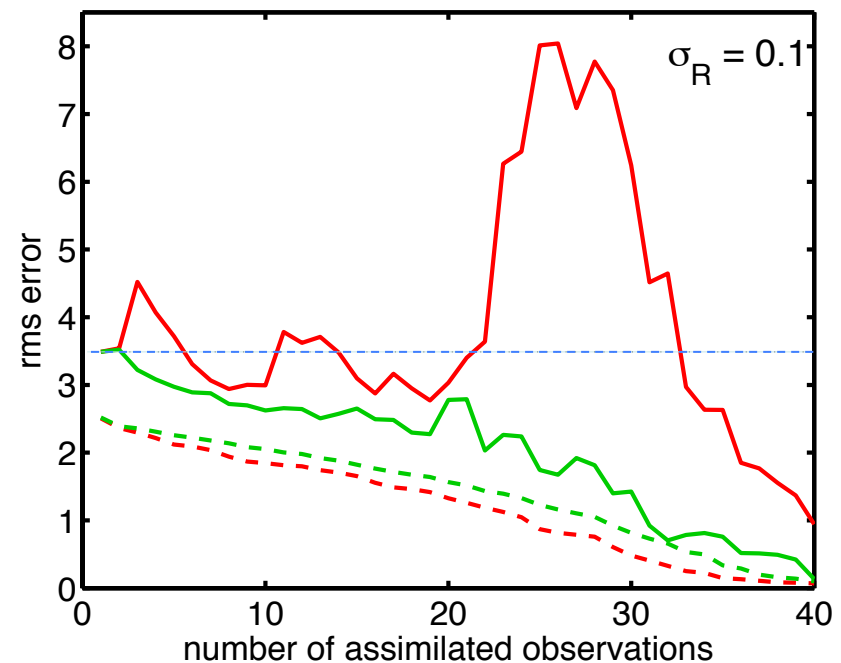
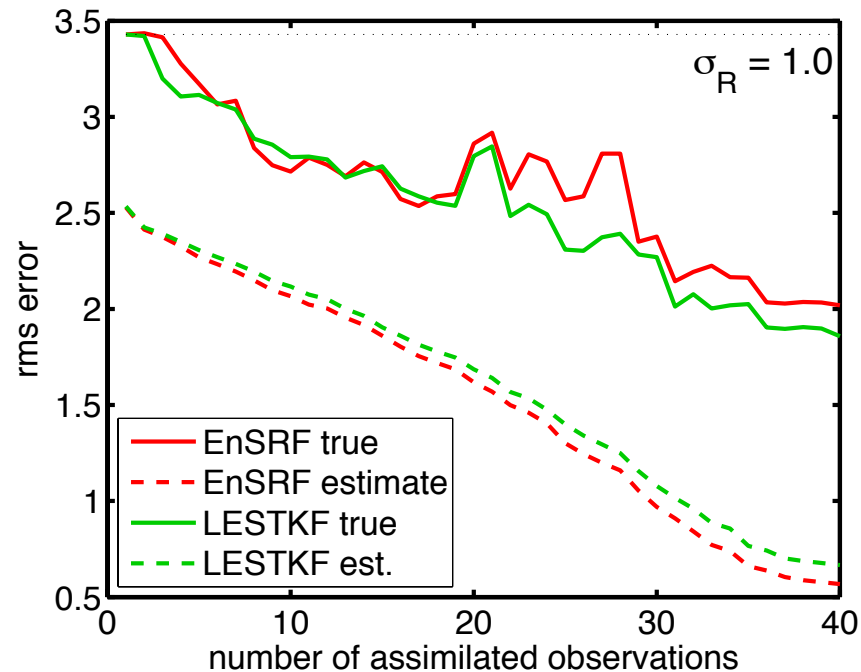


RMS error over number of observations

How does the RMS error develop during the loop over all observations?

At first analysis step:

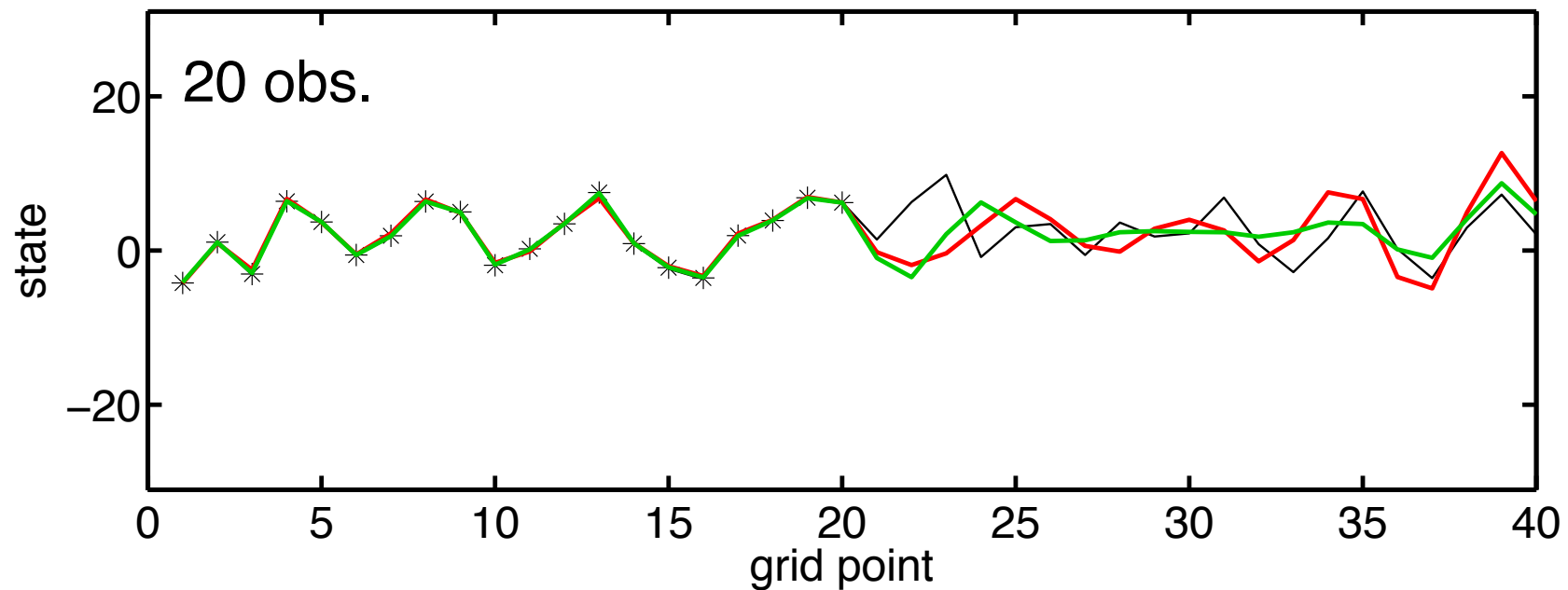
- EnSRF: Compute RMS errors at each iteration
- LESTKF: Do 40 experiments with increasing number of obs.



Instability of serial obs. Processing with localization

More detailed view:

- State estimate for different numbers of observations



Inconsistent matrix updates

The Kalman filter updates the covariance matrix according to

$$\mathbf{P}^a = (\mathbf{I} - \mathbf{K}\mathbf{H}) \mathbf{P}^f (\mathbf{I} - \mathbf{K}\mathbf{H})^T + \mathbf{K}\mathbf{R}\mathbf{K}^T \quad (1)$$

With the Kalman gain

$$\mathbf{K} = \mathbf{P}^f \mathbf{H}^T (\mathbf{H}\mathbf{P}^f \mathbf{H}^T + \mathbf{R})^{-1} \quad (2)$$

this simplifies to

$$\mathbf{P}^a = (\mathbf{I} - \mathbf{K}\mathbf{H}) \mathbf{P}^f \quad (3)$$

(1) and (3) yield same result **only** with gain (2)!

Not fulfilled with localization:

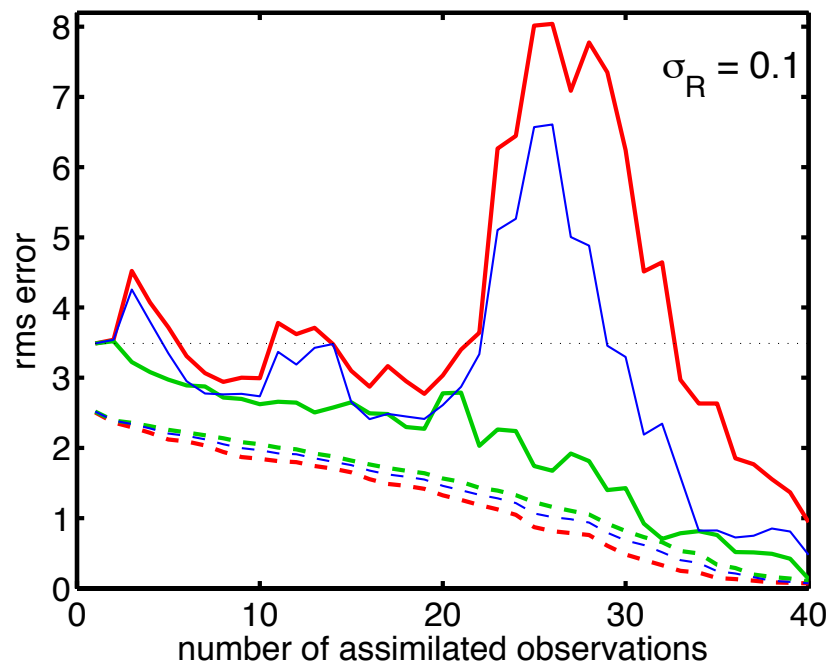
$$\mathbf{K}_{loc} = (\mathbf{C} \circ \mathbf{P}^f) \mathbf{H}^T (\mathbf{H} (\mathbf{C} \circ \mathbf{P}^f) \mathbf{H}^T + \mathbf{R})^{-1}$$

- Update of \mathbf{P} is inconsistent in localized EnSRF (already noted by Whitaker & Hamill (2002), but never further examined)

Inconsistent matrix updates (2)

The inconsistency also occurs in LETKF, LESTKF, LSEIK, EnKF ...

- But here: update is only done once followed by ensemble forecast
- LESTKF with serial observation processing also shows instability

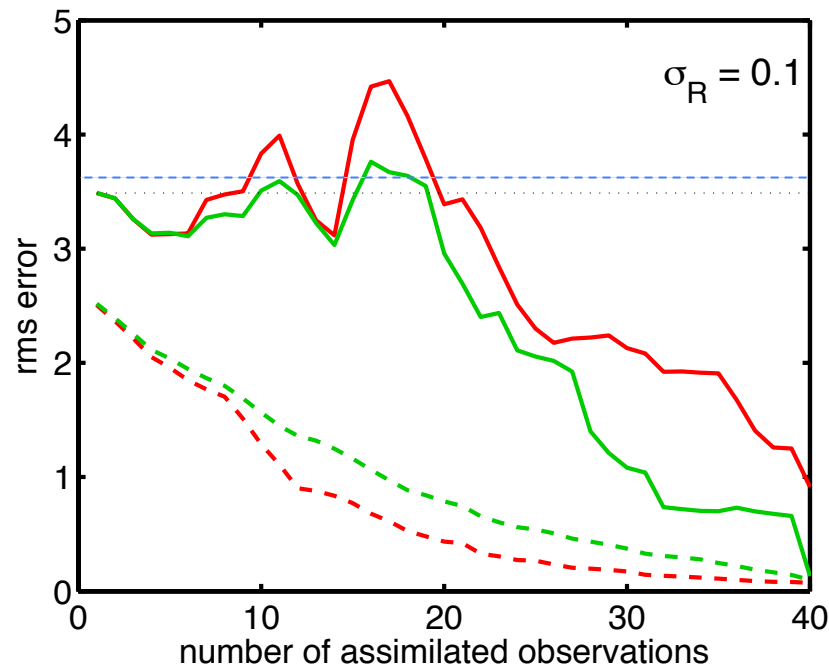


Blue: LESTKF
with serial
observation
processing

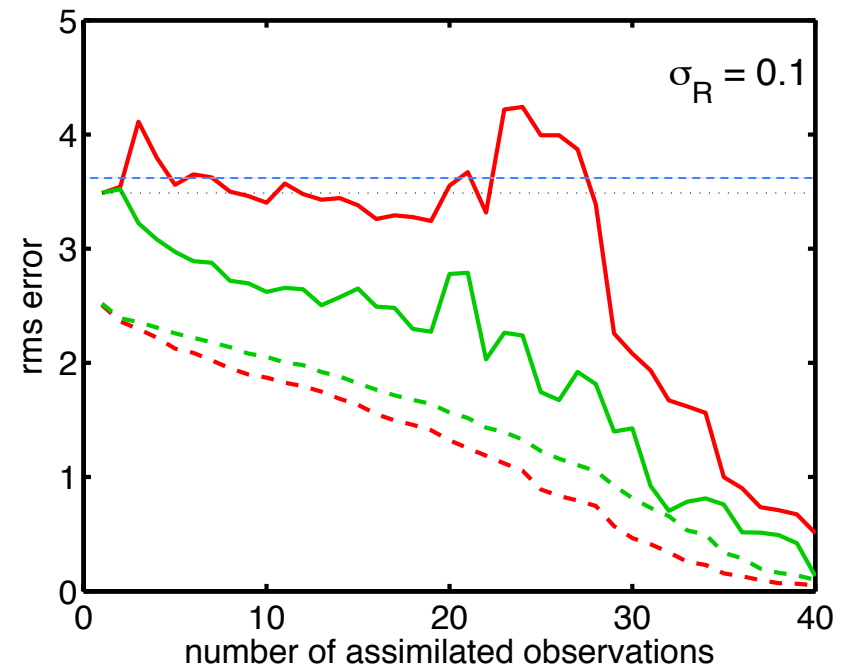
Effect of observation reordering

- Before: Assimilated observation from grid point 1 to 40 with increasing index
- What is the effect when we re-order the observations?

„maximum distance“
(1, 21, 11, 31, 6, 26,...)
EnSRF with re-ordered observations



local observation sorting
(Whitaker et al. 2008)
L-EnSRF and sorted observations



Serial obs. Processing and localization

- Update of covariance matrix is inconsistent
 - Because of asymmetric update equation
 - Because of small ensemble
 - Also the case for synchronous assimilation of observations (LETKF, LSEIK, LESTKF)

- Instability of serial observation processing
 - only significant when assimilation has strong influence (large state error and small observation error)
 - Can it happen, when ensemble spread gets large, e.g. due to ocean eddies, convection in atmosphere?

Summary

- Localization
 - is empirical
 - it works
 - regularizes the filter analysis step
 - does inconsistent covariance updates
- Optimal radius influenced by degrees of freedom from ensemble
- Interaction of localization and covariance matrix update still open

Thank you!